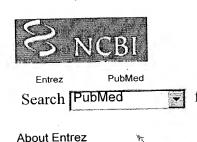
زري







| L | | 1 | of Medicine | | | |
|------------|---------|-----------|-------------|-----------|----------|---------|
| Nucleotide | Protein | Genome | Structure | PMC | Journals | Во |
| for | | | | Go Cle | | |
| Limits | Previev | v/Index l | History | Clipboard | | Details |
| | | - IS | 0 Sort | Ser | nd to Te | xt . |
| olav Abst | ract | Show: 2 | 0 Sort | 7 001 | | |

Text Version

Entrez PubMed Overview Help | FAQ Tutorial New/Noteworthy E-Utilities

PubMed Services
Journals Database
MeSH Database
Single Citation Matcher
Batch Citation Matcher
Clinical Queries
LinkOut
Cubby

Related Resources
Order Documents
NLM Gateway
TOXNET
Consumer Health
Clinical Alerts
ClinicalTrials.gov
PubMed Central

Privacy Policy

☐ 1: Biochemistry. 1997 Nov 4;36(44):13494-502.

Related Articles, Link



Dis

Nonpolar interactions of thrombin S' subsites with its bivalent inhibitor: methyl scan of the inhibitor linker.

Slon-Usakiewicz JJ, Purisima E, Tsuda Y, Sulea T, Pedyczak A, Fethiere J, Cygler M, Konishi Y.

National Research Council of Canada, Biotechnology Research Institute, Montreal, Quebec, Canada H4P 2R2.

We have designed bivalent thrombin inhibitors, consisting of a nonsubstrate type active site blocking segment, a hirudin-based fibrinogen recognition exosite blocking segment, and a linker connecting these segments. The inhibition provided by the bivalent inhibitors with various linker lengths revealed that a minimum of 15 atoms was required for simultaneous binding of the two blocking segments of the inhibitor to thrombin without significant distortion. The crystal structure of the inhibitors with a 16-atom linker showed some conformational flexibility in the linker portion which still lies deep in the groove joining the active site and the fibrinogen recognition exosite. Since the thrombin S' subsites are not well characterized, we designed a new strategy to search for possible nonpolar interactions between the linker and the thrombin S' subsites. This strategy, the "methyl scan", is based on the incorporation of a methyl side chain at each atom position of the linker by using sarcosine, D,L-alanine, D,L-3-aminoisobutyric acid, or Nmethyl-beta-alanine. The methyl groups on the second and the eighth atom positions of the linker, which correspond to the side chains of the P1' and the P3' residues, respectively, improved the affinity of the inhibitors significantly Further study of the stereospecificity showed that L-Ala at the P1' residue and D-Ala at the P3' residue preferably improved the affinity of the inhibitors 20and 25-fold, respectively. Molecular modeling calculations using a methyl probe were also carried out to identify favorable nonpolar interacting sites on the thrombin surface. Two sites were identified in the vicinity of the P1' and the P3' residues, supporting the validity of the methyl scan method. Thus, this study has improved our understanding of the interactions taking place in this groove. In particular, we have been able to show that some specific structural features, such as hydrophobic complementarity between the linker and the thrombin S' subsites, could be exploited and make these inhibitors trivalent.

=> fil reg FILE 'REGISTRY' ENTERED AT 09:45:13 ON 03 FEB 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

2 FEB 2004 HIGHEST RN 645336-91-0 STRUCTURE FILE UPDATES: 2 FEB 2004 HIGHEST RN 645336-91-0 DICTIONARY FILE UPDATES:

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> d sta que 110

82 SEA FILE=REGISTRY ABB=ON PLU=ON R'PIP'.G.G'BAL'DYEPIPEEAAE/SQ L8

82 SEA FILE=REGISTRY ABB=ON PLU=ON L8 AND PHENYL SULFONYL L10

=> d his

(FILE 'HOME' ENTERED AT 09:36:51 ON 03 FEB 2004) SET COST OFF

FILE 'HCAPLUS' ENTERED AT 09:37:15 ON 03 FEB 2004 E W097-CA745/AP, PRN

T.1 1 \$ E3,E4 SEL RN

FILE 'REGISTRY' ENTERED AT 09:37:37 ON 03 FEB 2004

L2 76 S E1-E76

75 S L2 AND 18/SQL

L3 75 S L3 AND 46.150.18/RID AND 46.150.1/RID L4

75 S L4 AND NC4/ES L_5

75 S L5 AND NC5/ES L6

75 S L6 AND NR>=6 1.7

82 S R'PIP'.G.G'BAL'DYEPIPEEAAE/SQSP 1.8

T. 9 7 S L8 NOT L7

82 S L8 AND PHENYL SULFONYL L10SAV L8 LIU529/A

FILE 'HCAOLD' ENTERED AT 09:42:00 ON 03 FEB 2004 0 S L10 L11

FILE 'HCAPLUS' ENTERED AT 09:42:06 ON 03 FEB 2004

L12 3 S L10

E KONISHI Y/AU

L13 283 S E3, E5, E14

E SLON J/AU

18 S E3-E7 L14

3 S L12 AND (KONISHI ? OR SLON ?)/AU L15

L16 3 S L12 AND L13, L14 L17 3 S L15, L16

FILE 'REGISTRY' ENTERED AT 09:44:31 ON 03 FEB 2004

L18 0 S L10 NOT D

L19 0 S L10 NOT 46.150.1/RID

FILE 'USPATFULL, USPAT2' ENTERED AT 09:44:51 ON 03 FEB 2004 L20 0 S L10

FILE 'REGISTRY' ENTERED AT 09:45:13 ON 03 FEB 2004

=> fil hcaplus FILE 'HCAPLUS' ENTERED AT 09:45:25 ON 03 FEB 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 AMERICAN CHEMICAL SOCIETY (ACS)

Copyright of the articles to which records in this database refer is held by the publishers listed in the PUBLISHER (PB) field (available for records published or updated in Chemical Abstracts after December 26, 1996), unless otherwise indicated in the original publications. The CA Lexicon is the copyrighted intellectual property of the the American Chemical Society and is provided to assist you in searching databases on STN. Any dissemination, distribution, copying, or storing of this information, without the prior written consent of CAS, is strictly prohibited.

FILE COVERS 1907 - 3 Feb 2004 VOL 140 ISS 6 FILE LAST UPDATED: 2 Feb 2004 (20040202/ED)

This file contains CAS Registry Numbers for easy and accurate substance identification.

=> d 117 all tot

- L17 ANSWER 1 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN
- AN 2000:94674 HCAPLUS
- DN 132:262009
- ED Entered STN: 10 Feb 2000
- TI Design of P1' and P3' Residues of Trivalent Thrombin Inhibitors and Their Crystal Structures
- AU Slon-Usakiewicz, Jacek J.; Sivaraman, J.; Li, Yunge; Cygler, Miroslaw; Konishi, Yasuo
- CS Biotechnology Research Institute, National Research Council of Canada, Montreal, QC, H4P 2R2, Can.
- SO Biochemistry (2000), 39(9), 2384-2391 CODEN: BICHAW; ISSN: 0006-2960
- PB American Chemical Society
- DT Journal
- LA English
- CC 7-3 (Enzymes)

Section cross-reference(s): 75

AB Synthetic bivalent thrombin inhibitors comprise an active site blocking segment, a fibrinogen recognition exosite blocking segment, and a linker connecting these segments. Possible nonpolar interactions of the P1' and P3' residues of the linker with thrombin S1' and S3' subsites, resp., were identified using the "Methyl Scan" method [Slon-Usakiewicz et al. (1997) Biochem. 36, 13494-13502]. A series of inhibitors (4-tert-butylbenzenesulfonyl)-Arg-(D-pipecolic acid)-Xaa-Gly-Yaa-Gly-βAla-Asp-Tyr-Glu-Pro-Ile-Pro-Glu-Glu-Ala-(β-cyclohexylalanine)-(D-Glu)-OH, in which nonpolar P1' residue Xaa or P3' residue Yaa was incorporated, were

```
designed and improved the affinity to thrombin. Substitution of the P3'
residue with D-phenylglycine or D-Phe improved the Ki value to (9.5 \pm
0.6) + 10-14 or 1.3 \pm 0.5 + 10-13 M, resp., compared to
that of a reference inhibitor with Gly residues at Xaa and Yaa residues (Ki =
(2.4 \pm 0.5) + 10-11 \text{ M}). Similarly, substitution of the P1'
residue with L-norleucine or L-\beta-(2-thienyl) alanine lowered the Ki
values to (8.2 \pm 0.6) + 10-14 or (5.1 \pm 0.4) + 10-14 M,
resp. The linker Gly-Gly-Gly-etaAla of the inhibitors in the previous
sentence was simplified with 12-aminododecanoic acid, resulting in further
improvement of the Ki values to (3.8 \pm 0.6) + 10-14 or (1.7 \pm
0.4) + 10-14 M, resp. These Ki values are equivalent to that of natural
hirudin (2.2 + 10-14 M), yet the size of the synthetic inhibitors (2
kD) is only one-third that of hirudin (7 kD). Two inhibitors, with
L-norleucine or L-\beta-(2-thienyl)alanine at the P1' residue and the
improved linker of 12-aminododecanoic acid, were crystallized in complex with
human \alpha-thrombin. The crystal structures of these complexes were
solved and refined to 2.1 Å resolution The Lys60F side chain of thrombin
moved significantly and formed a large nonpolar S1' subsite to accommodate
the bulky P1' residue.
trivalent thrombin inhibitor design crystal structure
Enzyme functional sites
   (active; design of P1' and P3' residues of trivalent thrombin
   inhibitors and their crystal structures)
Enzyme kinetics
   (of inhibition; design of P1' and P3' residues of trivalent thrombin
   inhibitors and their crystal structures)
Crystal structure
   (of trivalent thrombin inhibitors complexed with thrombin)
Structure-activity relationship
   (thrombin-inhibiting; design of P1' and P3' residues of trivalent
   thrombin inhibitors and their crystal structures)
9002-04-4D, Thrombin, complexes with trivalent thrombin inhibitors
263367-63-1D, complexes with thrombin 263367-64-2D, complexes with
thrombin
RL: PRP (Properties)
   (crystal structure; design of P1' and P3' residues of trivalent
   thrombin inhibitors and their crystal structures)
197518-05-1 197518-06-2 197518-07-3
197518-08-4 197519-06-5 223117-53-1
223117-64-4 223117-70-2 223117-75-7
223117-81-5 223117-89-3 223117-95-1
223118-14-7 223118-20-5 223118-31-8
223118-41-0 223118-52-3 223118-59-0
223118-64-7 223118-70-5 223118-76-1
223118-82-9 223118-88-5 223119-00-4
223119-13-9 223119-22-0 223119-28-6
223119-36-6 223119-45-7 223119-53-7
223119-62-8 223119-72-0 223119-78-6
223119-87-7 223119-93-5 223120-02-3
223120-12-5 223120-26-1 223120-49-8
223120-63-6 223120-68-1 223120-74-9
223120-84-1 223120-90-9 223120-97-6
223121-11-7 223121-17-3 223121-22-0
223121-31-1 223121-36-6 223121-41-3
223121-48-0 223121-54-8 223121-58-2
223121-63-9 223121-68-4 223121-74-2
223121-88-8 223121-94-6 223122-01-8
223122-06-3 223122-18-7 223122-23-4
223122-27-8 223122-31-4 223122-37-0
223122-44-9 223122-52-9 223122-63-2
223122-72-3 223122-83-6 263367-65-3
                                                         263367-70-0
               263367-67-5
                             263367-68-6
                                           263367-69-7
263367-66-4
```

SŢ

IT

IT

IT

IT

IT

ΙT

263367-74-4

RE

L17

ANDN

ED

TΙ

IN PΑ

SO

DT

PCT Int. Appl., 46 pp.

CODEN: PIXXD2

Patent

```
RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); PRP (Properties); BIOL (Biological study)
        (design of P1' and P3' residues of trivalent thrombin inhibitors and
        their crystal structures)
     9002-04-4, Thrombin
     RL: BPR (Biological process); BSU (Biological study, unclassified); PRP
     (Properties); BIOL (Biological study); PROC (Process)
        (design of P1' and P3' residues of trivalent thrombin inhibitors and
        their crystal structures)
              THERE ARE 39 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE.CNT
        39
(1) Blomback, B; Nature 1967, V215, P1445 HCAPLUS
(2) Bode, W; EMBO J 1989, V8, P3467 HCAPLUS
(3) Bourdon, P; FEBS Lett 1991, V294, P163 HCAPLUS
(4) Brunger, A; X-plor version 3.1 1993
(5) Charles, R; J Med Chem 1999, V42, P1376
(6) Dimaio, J; FEBS Lett 1991, V282, P47 HCAPLUS
(7) Dimaio, J; J Biol Chem 1990, V265, P21698 HCAPLUS
(8) Dimaio, J; J Med Chem 1992, V35, P3331 HCAPLUS
(9) Fethiere, J; Protein Sci 1996, V5, P1174 HCAPLUS
(10) Jones, T; Acta Crstallogr 1991, VA47, P110 HCAPLUS
(11) Kline, T; Biochem Biophys Res Commun 1991, V177, P1049 HCAPLUS
(12) Krishnan, R; Protein Sci 1996, V5, P422 HCAPLUS
(13) Laudano, A; Ann N Y Acad Sci 1983, V27, P315
(14) Le Bonniec, B; Biochemistry 1996, V35, P7114 HCAPLUS
(15) Lombardi, A; J Med Chem 1996, V39, P2008 HCAPLUS
(16) Lombardi, A; Protein Sci 1999, V8, P91 HCAPLUS
(17) Maraganore, J; Biochemistry 1990, V29, P7095 HCAPLUS
(18) Martin, P; J Biol Chem 1992, V267, P7911 HCAPLUS
(19) Matthews, J; Biophys J 1996, V71, P2830 HCAPLUS
(20) Minor, W; XDISPLAY 1993
(21) Okuyama, K; Biopolymers 1996, V40, P85 HCAPLUS
(22) Otwinowski, Z; Proceedings of the CCP4 Study Weekend: Data Collection and
    Processing 1993, P56
(23) Qiu, X; Biochemistry 1992, V31, P11689 HCAPLUS
(24) Rehse, P; Biochemistry 1995, V34, P11537 HCAPLUS
(25) Rezaie, A; Biochemistry 1997, V36, P1026 HCAPLUS
(26) Schechter, I; Biochem Biophys Res Commun 1967, V27, P157 HCAPLUS
(27) Segel, I; Enzyme Kinetics: Behawior and Analysis of Rapid Equilibrium and
    Steady-State Enzyme Systems 1975, P100
(28) Skordalakes, E; Biochemistry 1998, V37, P14420 HCAPLUS
(29) Skrzypczak-Jankun, E; J Mol Biol 1991, V221, P1379 HCAPLUS
(30) Slon-Usakiewicz, J; Biochemistry 1997, V36, P13494 HCAPLUS
(31) Stephens, A; J Biol Chem 1988, V263, P3639
(32) Stubbs, M; Thrombin Res 1993, V69, P1 HCAPLUS
(33) Szewczuk, Z; Biochemistry 1992, V31, P9132 HCAPLUS
(34) Szewczuk, Z; Biochemistry 1993, V32, P3396 HCAPLUS
(35) Theunissen, H; J Biol Chem 1993, V268, P9035 HCAPLUS
(36) Tsuda, Y; Biochemistry 1994, V33, P14443 HCAPLUS
(37) Vu, T; Cell 1991, V64, P1057 HCAPLUS
(38) Wnendt, S; Protein Eng 1997, V10, P169 HCAPLUS
(39) Zdanov, A; Proteins 1993, V17, P252 HCAPLUS
    ANSWER 2 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN
     1999:271384 HCAPLUS
     130:297001
     Entered STN: 03 May 1999
     Preparation of trivalent thrombin inhibitors
     Konishi, Yasuo; Slon, Jacek
     National Research Council of Canada, Can.
```

```
LA
     English
     ICM C07K014-815
IC
         A61K038-58
     34-3 (Amino Acids, Peptides, and Proteins)
     Section cross-reference(s): 1, 7
FAN.CNT 1
     PATENT NO.
                      KIND
                            DATE
                                           APPLICATION NO.
                      ____
                                           WO 1997-CA745
                            19990422
PI
     WO 9919356
                      Α1
         W: AL, AM, AT, AU, AZ, BA, BB, BG, BR, BY, CA, CH, CN, CU, CZ, DE,
             DK, EE, ES, FI, GB, GE, GH, HU, ID, IL, IS, JP, KE, KG, KP, KR,
             KZ, LC, LK, LR, LS, LT, LU, LV, MD, MG, MK, MN, MW, MX, NO, NZ,
             PL, PT, RO, RU, SD, SE, SG, SI, SK, SL, TJ, TM, TR, TT, UA, UG,
             US, UZ, VN, YU, ZW, AM, AZ, BY, KG, KZ, MD, RU, TJ, TM
         RW: GH, KE, LS, MW, SD, SZ, UG, ZW, AT, BE, CH, DE, DK, ES, FI, FR,
             GB, GR, IE, IT, LU, MC, NL, PT, SE, BF, BJ, CF, CG, CI, CM, GA,
             GN, ML, MR, NE, SN, TD, TG
     AU 9746122
                            19990503
                                           AU 1997-46122
                                                             19971015
                       Α1
     AU 761011
                            20030529
                       B2
                                           EP 1997-944656
                                                             19971015
     EP 1023324.
                            20000802
                       A1
            AT, BE, CH, DE, DK, ES, FR, GB, GR, IT, LI, LU, NL, SE, MC, PT,
             IE, FI
                            20010928
                                           NZ 1997-503669
                                                             19971015
     NZ 503669
                       Α
     JP 2001519442
                       T2
                            20011023
                                            JP 2000-515927
                                                             19971015
PRAI WO 1997-CA745
                       Α
                            19971015
     MARPAT 130:297001
OS
     Trivalent thrombin inhibitors AS-Z-P (AS represents an S subsite blocking
AΒ
     segment, P represents a fibrinogen recognition exosite blocking segment, Z
     represents a S' subsite blocking segment) or their pharmaceutically
     acceptable salts, were prepared The S' subsite blocking segment, besides
     binding to the thrombin S' subsites, connects the S subsite blocking
     segment and the fibrinogen recognition exosite blocking segment. This
     binding of Z segment together with the bindings of the AS and P segments,
     contributes to improve the affinity of the inhibitors significantly.
     AS blocking segment and the P segment preferably have the sequence
     Bbs-Arg-D-Pip- (Bbs = 4-tert-butylbenzenesulfonyl, Pip = pipecolic acid)
     and Asp-Tyr-Glu-Pro-Ile-Pro-Glu-Glu-Ala-Cha-D-Glu-OH (Cha =
     \beta-cyclohexylalanine), resp. The Z segment preferably has the
     sequence Xaa-Gly-Yaa-Gly-\beta-Ala where: Xaa, Yaa = Gly, Ala, D-Ala,
     Val, D-Val, Phe, D-Phe, His, D-His, Nva, D-Nva, Ile, D-Ile, Nle, D-Nle,
     lphaAib (2-aminoisobutyric acid), Phg (phenylglycine), D-Phg, Thi
     (\beta-(2-\text{thienyl})\text{alanine}), D-Thi, Chq (cyclohexylglycine), etc. Thus,
     Bbs-Arg-D-Pip-Thi-Gly-Gly-Gly-β-Ala-Asp-Tyr-Glu-Pro-Ile-Pro-Glu-Glu-
     Ala-Cha-D-Glu-OH, having a Ki value of 0.051 \pm 0.004 pM, was prepared by
     the solid phase method using a conventional Fmoc procedure. The preferred
     inhibitors have Ki values smaller the 1 pM and are useful for treating or
     preventing vascular diseases.
     peptide prepn trivalent thrombin inhibitor
ST
     Peptides, preparation
ΙT
     RL: BAC (Biological activity or effector, except adverse); BSU (Biological
     study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
     BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of trivalent thrombin inhibitors)
     Blood vessel, disease
IT
        (treatment of; preparation of trivalent thrombin inhibitors)
     9002-04-4, Thrombin
IT
     RL: BSU (Biological study, unclassified); BIOL (Biological study)
        (inhibitors; preparation of trivalent thrombin inhibitors)
IT
     197518-05-1P 197518-06-2P 197518-07-3P
     197518-08-4P 197519-06-5P 223117-53-1P
     223117-64-4P 223117-70-2P 223117-75-7P
     223117-81-5P 223117-89-3P 223117-95-1P
     223118-04-5P 223118-14-7P 223118-20-5P
```

```
223118-31-8P 223118-41-0P 223118-52-3P
    223118-59-0P 223118-64-7P 223118-70-5P
    223118-76-1P 223118-82-9P 223118-88-5P
    223119-00-4P 223119-07-1P 223119-13-9P
    223119-22-0P 223119-28-6P 223119-36-6P
    223119-45-7P 223119-53-7P 223119-62-8P
    223119-72-0P 223119-78-6P 223119-87-7P
    223119-93-5P 223120-02-3P 223120-12-5P
    223120-26-1P 223120-49-8P 223120-63-6P
    223120-68-1P 223120-74-9P 223120-84-1P
    223120-90-9P 223120-97-6P 223121-04-8P
    223121-11-7P 223121-17-3P 223121-22-0P
    223121-31-1P 223121-36-6P 223121-41-3P
    223121-48-0P 223121-54-8P 223121-58-2P
    223121-63-9P 223121-68-4P 223121-74-2P
    223121-81-1P 223121-88-8P 223121-94-6P
    223122-01-8P 223122-06-3P 223122-18-7P
    223122-23-4P 223122-27-8P 223122-31-4P
    223122-37-0P 223122-44-9P 223122-52-9P
    223122-63-2P 223122-72-3P 223122-83-6P
    RL: BAC (Biological activity or effector, except adverse); BSU (Biological
    study, unclassified); SPN (Synthetic preparation); THU (Therapeutic use);
    BIOL (Biological study); PREP (Preparation); USES (Uses)
        (preparation of trivalent thrombin inhibitors)
     9002-04-4, Thrombin
     RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL
     (Biological study); PROC (Process)
        (\alpha-; preparation of trivalent thrombin inhibitors)
              THERE ARE 4 CITED REFERENCES AVAILABLE FOR THIS RECORD
RE.CNT
(1) Konishi, Y; WO 9511921 A 1995 HCAPLUS
(2) Krishnan; PROTEIN SCIENCE 1996, V5(3), P422 HCAPLUS
(3) Szewczuk, E; BIOCHEMISTRY 1993, V32(13), P3396
(4) Tsuda, E; BIOCHEMISTRY 1994, V33(48), P14443
    ANSWER 3 OF 3 HCAPLUS COPYRIGHT 2004 ACS on STN
     1997:660911
                 HCAPLUS
     127:316126
     Entered STN: 18 Oct 1997
     Nonpolar interactions of thrombin S' subsites with its bivalent inhibitor:
    methyl scan of the inhibitor linker
     Slon-Usakiewicz, Jacek J.; Purisima, Enrico; Tsuda, Yuko; Sulea,
    Traian; Pedyczak, Artur; Fethiere, James; Cygler, Miroslaw; Konishi,
     Yasuo
     National Research Council of Canada, Biotechnology Research Institute,
    Montreal, QC, H4P 2R2, Can.
     Biochemistry (1997), 36(44), 13494-13502
     CODEN: BICHAW; ISSN: 0006-2960
     American Chemical Society
     Journal
     English
     7-3 (Enzymes)
     We have designed bivalent thrombin inhibitors, consisting of a
     nonsubstrate type active site blocking segment, a hirudin-based fibrinogen
     recognition exosite blocking segment, and a linker connecting these
     segments. The inhibition provided by the bivalent inhibitors with various
     linker lengths revealed that a min. of 15 atoms was required for
     simultaneous binding of the two blocking segments of the inhibitor to
     thrombin without significant distortion. The crystal structure of the
     inhibitors with a 16-atom linker showed some conformational flexibility in
     the linker portion which still lies deep in the groove joining the active
```

site and the fibrinogen recognition exosite. Since the thrombin S'

subsites are not well characterized, we designed a new strategy to search

IT

RE

ΑN DN

ED

TΙ

ΑU

CS

SO

PB

DT

LA CC

AB

for possible nonpolar interactions between the linker and the thrombin S' subsites. This strategy, the "methyl scan", is based on the incorporation of a Me side chain at each atom position of the linker by using sarcosine, D,L-alanine, D,L-3-aminoisobutyric acid, or N-methyl- β -alanine. The Me groups on the second and the eighth atom positions of the linker, which correspond to the side chains of the P1' and the P3' residues, resp., improved the affinity of the inhibitors significantly. Further study of the stereospecificity showed that L-Ala at the P1' residue and D-Ala at the P3' residue preferably improved the affinity of the inhibitors 20- and 25-fold, resp. Mol. modeling calcns. using a Me probe were also carried out to identify favorable nonpolar interacting sites on the thrombin surface. Two sites were identified in the vicinity of the P1' and the P3' residues, supporting the validity of the Me scan method. Thus, this study has improved our understanding of the interactions taking place in this groove. In particular, we have been able to show that some specific structural features, such as hydrophobic complementarity between the linker and the thrombin S' subsites, could be exploited and make these inhibitors trivalent. thrombin inhibitor peptide bivalent interaction

ST

TT Methyl group

> (Me scan method; nonpolar interactions of thrombin S' subsites with its bivalent inhibitor: Me scan of inhibitor linker)

ΤТ Enzyme functional sites

Molecular association

(nonpolar interactions of thrombin S' subsites with its bivalent inhibitor: Me scan of inhibitor linker)

ITEnzyme kinetics

> RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(of inhibition; nonpolar interactions of thrombin S' subsites with its bivalent inhibitor: Me scan of inhibitor linker)

Crystal structure ΙT

> (of thrombin-substrate; nonpolar interactions of thrombin S' subsites with its bivalent inhibitor: Me scan of inhibitor linker)

ΙT

ΙT

(protein, of thrombin-substrate; nonpolar interactions of thrombin S' subsites with its bivalent inhibitor: Me scan of inhibitor linker) Peptides, biological studies

RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(thrombin inhibitor; nonpolar interactions of thrombin S' subsites with its bivalent inhibitor: Me scan of inhibitor linker)

ΙT 159218-12-9 159218-18-5 170429-33-1 170429-34-2 170429-35-3 170429-36-4 170429-37-5 170429-38-6 170429-39-7 170429-40-0 170429-43-3 197518-01-7 197518-02-8 197518-03-9 197518-04-0 197518-05-1

RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(as thrombin inhibitor; nonpolar interactions of thrombin S' subsites with its bivalent inhibitor: Me scan of inhibitor linker)

197518-06-2 197518-07-3 197518-08-4 TT 197518-09-5

197518-10-8 **197518-11-9 197518-12-0** 197518-13-1 197518-14-2 197518-15-3 197518-16-4 **197518-17-5**

197518-19-7 197518-21-1 197518-23-3 197518-24-4

197518-29-9 197518-26-6 **197518-27-7** 197518-28-8

197518-31-3 197518-32-4 197518-33-5 197518-34-6 197518-36-8

197518-38-0 197518-39-1 197518-40-4 197519-06-5

197717-04-7 197717-09-2 197717-13-8 197717-14-9 197717-16-1 197717-17-2

RL: BAC (Biological activity or effector, except adverse); BPR (Biological process); BSU (Biological study, unclassified); BUU (Biological use,

unclassified); BIOL (Biological study); PROC (Process); USES (Uses) (as thrombin inhibitor; nonpolar interactions of thrombin S' subsites with its bivalent inhibitor: Me scan of inhibitor linker) 107-97-1, Sarcosine 144-90-1, 3-Aminoisobutyric acid 302-72-7, dl-Alanine 2679-14-3, N-Methyl-β-alanine.

RL: BUU (Biological use, unclassified); BIOL (Biological study); USES (Uses)

(in Me scan method; nonpolar interactions of thrombin S' subsites with its bivalent inhibitor: Me scan of inhibitor linker)

IT 9002-04-4, Thrombin

IT

RL: BSU (Biological study, unclassified); BIOL (Biological study) (inhibitors; nonpolar interactions of thrombin S' subsites with its bivalent inhibitor: Me scan of inhibitor linker)

IT 9002-04-4, Thrombin

RL: BPR (Biological process); BSU (Biological study, unclassified); BIOL (Biological study); PROC (Process)

(nonpolar interactions of thrombin S' subsites with its bivalent inhibitor: Me scan of inhibitor linker)

IT 56-41-7, Alanine, biological studies

RL: BSU (Biological study, unclassified); BIOL (Biological study) (of thrombin; nonpolar interactions of thrombin S' subsites with its bivalent inhibitor: Me scan of inhibitor linker)

=> fil reg FILE 'REGISTRY' ENTERED AT 09:45:40 ON 03 FEB 2004 USE IS SUBJECT TO THE TERMS OF YOUR STN CUSTOMER AGREEMENT. PLEASE SEE "HELP USAGETERMS" FOR DETAILS. COPYRIGHT (C) 2004 American Chemical Society (ACS)

Property values tagged with IC are from the ZIC/VINITI data file provided by InfoChem.

STRUCTURE FILE UPDATES: 2 FEB 2004 HIGHEST RN 645336-91-0 DICTIONARY FILE UPDATES: 2 FEB 2004 HIGHEST RN 645336-91-0

TSCA INFORMATION NOW CURRENT THROUGH JULY 14, 2003

Please note that search-term pricing does apply when conducting SmartSELECT searches.

Crossover limits have been increased. See HELP CROSSOVER for details.

Experimental and calculated property data are now available. For more information enter HELP PROP at an arrow prompt in the file or refer to the file summary sheet on the web at: http://www.cas.org/ONLINE/DBSS/registryss.html

=> d l10 ide can tot

L10 ANSWER 1 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 263367-74-4 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-(2S)-2-cyclohexylglycylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

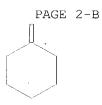
MF C100 H149 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

^{**}RELATED SEQUENCES AVAILABLE WITH SEQLINK**

Absolute stereochemistry.



1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

L10 ANSWER 2 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 263367-65-3 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-(2S)-2-cyclohexylglycylglycylglycylglycylglycylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C100 H149 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

`**RELATED SEQUENCES AVAILABLE WITH SEQLINK**

PAGE 2-C



1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

L10 ANSWER 3 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223122-83-6 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-3-(2-thienyl)-D-alanylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C99 H143 N21 O32 S2

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

PAGE 1-A

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE

1: 132:262009

REFERENCE

2: 130:297001

L10 ANSWER 4 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223122-72-3 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-3-(2-thienyl)-L-alanylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C99 H143 N21 O32 S2

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

PAGE 1-A

PAGE 1-C

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE

1: 132:262009

REFERENCE

2: 130:297001

L10 ANSWER 5 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223122-63-2 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-D-tryptophylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-

alanyl- (9CI) (CA INDEX NAME) PROTEIN SEQUENCE; STEREOSEARCH C103 H146 N22 O32 S

FS

MF

SR CA

LCSTN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

PAGE 2-C

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 6 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223122-52-9 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-L-tryptophylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C103 H146 N22 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

PAGE 2-C

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 7 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223122-44-9 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-D-histidylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C98 H143 N23 O32 S

SR CF

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

PAGE 1-A

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE

1: 132:262009

REFERENCE

2: 130:297001

L10 ANSWER 8 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223122-37-0 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-L-histidylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C98 H143 N23 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

PAGE 1-A

PAGE 1-C

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

: 132:262009

REFERENCE

2: 130:297001

L10 ANSWER 9 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223122-31-4 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-(αR)-α-aminobenzenebutanoylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-α-glutamyl-L-NDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C102 H147 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE

1: 132:262009

REFERENCE

2: 130:297001

L10 ANSWER 10 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223122-27-8 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-(αS)-α-aminobenzenebutanoylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C102 H147 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

PAGE 1-A

PAGE 1-C

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE

1: 132:262009

REFERENCE

2: 130:297001

L10 ANSWER 11 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223122-23-4 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-D-phenylalanylglycyl- β -alanyl-L- α -aspartyl-L-tyrosyl-L- α -glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L- α -glutamyl-L-alanyl-3-cyclohexyl-L-

alanyl- (9CI) (CA INDEX NAME) PROTEIN SEQUENCE; STEREOSEARCH C101 H145 N21 O32 S

FS

MF

SR CA

LCSTN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 12 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223122-18-7 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-L-phenylalanylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C101 H145 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE

1: 132:262009

REFERENCE

2: 130:297001

L10 ANSWER 13 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223122-06-3 REGISTRÝ

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-(2R)-2-phenylglycylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C100 H143 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE

1: 132:262009

REFERENCE

2: 130:297001

L10 ANSWER 14 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223122-01-8 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-(2S)-2-phenylglycylglycyl- β -alanyl-L- α -aspartyl-L-tyrosyl-L- α -glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L- α -glutamyl-L- α -glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C100 H143 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

y garde

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE

1: 132:262009

REFERENCE

2: 130:297001

L10 ANSWER 15 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223121-94-6 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-3-cyclohexyl-D-alanylglycyl- β -alanyl-L- α -aspartyl-L-tyrosyl-L- α -glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L- α -glutamyl-L- α -glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C101 H151 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

PAGE 1-A

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 16 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223121-88-8 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-3-cyclohexyl-L-alanylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C101 H151 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

PAGE 1-A

HO2C R CO2H

O NH O HO2C O H NH S N H

PAGE 1-C

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 17 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223121-81-1 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-2-cyclohexylglycylglycyl- β -alanyl-L- α -aspartyl-L-tyrosyl-L- α -glutamyl-L-prolyl-L-

isoleucyl-L-prolyl-L- α -glutamyl-L- α -glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME) PROTEIN SEQUENCE; STEREOSEARCH C100 H149 N21 O32 S

FS

MF

SR

STN Files: LCCA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

PAGE 2-B

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:297001

L10 ANSWER 18 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223121-74-2 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-D-leucylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C98 H147 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 19 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223121-68-4 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-L-leucylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C98 H147 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

PAGE 1-A

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE

1: 132:262009

REFERENCE

2: 130:297001

L10 ANSWER 20 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223121-63-9 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-D-isoleucylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C98 H147 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

L: 132:262009

REFERENCE

2: 130:297001

L10 ANSWER 21 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223121-58-2 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-L-isoleucylglycyl- β -alanyl-L- α -aspartyl-L-tyrosyl-L- α -glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-a-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C98 H147 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 22 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223121-54-8 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-3-methyl-D-valylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-

alanyl- (9CI) (CA INDEX NAME)
S PROTEIN SEQUENCE; STEREOSEARCH

FS PROTEIN SEQUENCE; STI MF C98 H147 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

PAGE 1-A

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE

1: 132:262009

REFERENCE

2: 130:297001

L10 ANSWER 23 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223121-48-0 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-3-methyl-L-valylglycyl- β -alanyl-L- α -aspartyl-L-tyrosyl-L- α -glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-a-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C98 H147 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 24 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223121-41-3 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-D-valylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C97 H145 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

ANSWER 25 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN L10

RN 223121-36-6 REGISTRY

CND-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R) -2-piperidinecarbonylglycylglycyl-L-valylglycyl-\(\beta\)-alanyl-L- $\alpha \hbox{-aspartyl-$L$-tyrosyl-$L$-$\alpha$-glutamyl-$L$-prolyl-$L$-isoleucyl-$L$-}$ alanyl- (9CI) (CA INDEX NAME)

PROTEIN SEQUENCE; STEREOSEARCH FS

C97 H145 N21 O32 S MF

SR

LCSTN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE

1: 132:262009

REFERENCE

2: 130:297001

L10 ANSWER 26 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223121-31-1 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-D-methionylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C97 H145 N21 O32 S2

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

PAGE 1-A

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE

1: 132:262009

REFERENCE

2: 130:297001

L10 ANSWER 27 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223121-22-0 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-L-methionylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C97 H145 N21 O32 S2

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

PAGE 1-A

HO2C
R
CO2H
O
NH
O
HO2C
S
N
H
S
N
H
S
N
H
S
N
H
S
N
H
S
Me
Et

PAGE 1-C

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 28 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223121-17-3 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-3-mercapto-D-valylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

PROTEIN SEQUENCE; STEREOSEARCH C97 H145 N21 O32 S2 FS

MF

SR

LCSTN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 29 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223121-11-7 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-3-mercapto-L-valylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C97 H145 N21 O32 S2

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

PAGE 1-A

S Et

Ме

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE

1: 132:262009

REFERENCE

2: 130:297001

L10 ANSWER 30 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223121-04-8 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-L-cysteinylglycyl- β -alanyl-L- α -aspartyl-L-tyrosyl-L- α -glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L- α -glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C95 H141 N21 O32 S2

SR CA

LC STN Files: CA, CAPLUS

Absolute stereochemistry.

HO2C R CO2H

O NH
O HO2C
S N
H
Me
O HO2C
S N
H
N

PAGE 1-C

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:297001

L10 ANSWER 31 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223120-97-6 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-D-norleucylglycyl- β -alanyl-L- α -aspartyl-L-tyrosyl-L- α -glutamyl-L-prolyl-L-isoleucyl-L-

prolyl-L- α -glutamyl-L- α -glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME) PROTEIN SEQUENCE; STEREOSEARCH

FS

MFC98 H147 N21 O32 S

SR

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE

1: 132:262009

REFERENCE

2: 130:297001

L10 ANSWER 32 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223120-90-9 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-L-norleucylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C98 H147 N21 O32.S

SR CF

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

PAGE 1-A

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1

1: 132:262009

REFERENCE

2: 130:297001

L10 ANSWER 33 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223120-84-1 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-D-norvalylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C97 H145 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

PAGE 1-A

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE

1: 132:262009

REFERENCE

2: 130:297001

L10 ANSWER 34 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223120-74-9 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-L-norvalylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

PROTEIN SEQUENCE; STEREOSEARCH

FS PROTEIN SEQUENCE; S MF C97 H145 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

PAGE 1-A

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 35 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223120-68-1 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-(2R)-2-aminobutanoylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C96 H143 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

PAGE 1-A

PAGE 1-B

.

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE

1: 132:262009

REFERENCE

2: 130:297001

L10 ANSWER 36 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223120-63-6 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-(2S)-2-aminobutanoylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C96 H143 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

PAGE 1-A

PAGE 1-A

Et

Ме

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE

1: 132:262009

REFERENCE

2: 130:297001

L10 ANSWER 37 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223120-49-8 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-2-methylalanylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-1-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-1-alanyl-3-cyclohexyl-1-alanyl-3-cyclohexyl-1-alanyl-3-cyclohexyl-1-alanyl-3-cyclohexyl-1-alanyl-3-cyclohexyl-1-alanyl-3-cyclohexyl-1-alanyl-3-cyclohexyl-1-alanyl-3-cyclohexyl-1-alanyl-3-cyclohexyl-1-alanyl-3-cyclohexyl-1-alanyl-3-cyclohexyl-1-alanyl-3-cyclohexyl-1-alanyl-3-cyclohexyl-

alanyl- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C96 H143 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

$$HO_2C$$
 NH
 O
 HO_2C
 H
 S
 H
 S
 H
 S
 H
 S
 H
 M
 S
 H
 S

PAGE 1-C

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 38 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223120-26-1 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-

(2R)-2-piperidinecarbonyl-3-(2-thienyl)-D-alanylglycylglycylglycyl- β -alanyl-L- α -aspartyl-L-tyrosyl-L- α -glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L- α -glutamyl-L- α -glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C99 H143 N21 O32 S2

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE

1: 132:262009

REFERENCE

2: 130:297001

L10 ANSWER 39 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223120-12-5 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-3-(2-thienyl)-L-alanylglycylglycylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C99 H143 N21 O32 S2

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE

1: 132:262009

REFERENCE

2: 130:297001

L10 ANSWER 40 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223120-02-3 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-D-tryptophylglycylglycylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C103 H146 N22 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

PAGE 1-A

PAGE 2-C

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

130:297001 REFERENCE

L10 ANSWER 41 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN RN 223119-93-5 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-L-tryptophylglycylglycylglycylglycyl- β -alanyl-L- α -aspartyl-L-tyrosyl-L- α -glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L- α -glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C103 H146 N22 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

PAGE 1-A

PAGE 2-C

2 REFERENCES IN FILE CA (1907 TO DATE) 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

2: 130:297001 REFERENCE

L10 ANSWER 42 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223119-87-7 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-D-histidylglycylglycylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C98 H143 N23 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

PAGE 1-A

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE

1: 132:262009

REFERENCE

2: 130:297001

L10 ANSWE

ANSWER 43 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223119-78-6 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-L-histidylglycylglycylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(CA INDEX NAME)

alanyl- (9CI) (CA INDEX NAME) PROTEIN SEQUENCE; STEREOSEARCH

MF C98 H143 N23 O32 S

SR CA.

FS

LC STN Files:

CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

PAGE 1-A

PAGE 1-C

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 44 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223119-72-0 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-(α R)- α -aminobenzenebutanoylglycylglycylglycylglycylglycyl- β -alanyl-L- α -aspartyl-L-tyrosyl-L- α -glutamyl-L-prolyl-L- α -glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C102 H147 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

PAGE 1-C

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 45 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223119-62-8 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-(α S)- α -aminobenzenebutanoylglycylglycylglycylglycylglycyl- β -alanyl-L- α -aspartyl-L-tyrosyl-L- α -glutamyl-L-prolyl-L- α -glutamyl-L-alanyl-prolyl-L-isoleucyl-L-prolyl-L- α -glutamyl-L-alanyl-

3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C102 H147 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE

1: 132:262009

REFERENCE

2: 130:297001

L10 ANSWER 46 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223119-53-7 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-D-phenylalanylglycylglycylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C101 H145 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

PAGE 1-C

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 47 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

223119-45-7 REGISTRY RN

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-L-phenylalanylglycylglycylglycyl- β -alanyl-L- α -aspartyl-L-tyrosyl-L- α -glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L- α -glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C101 H145 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 48 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223119-36-6 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-(2R)-2-phenylglycylglycylglycylglycylglycylglycylglycylglycylglycylglycylglycylglycylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C100 H143 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 49 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223119-28-6 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-(2S)-2-phenylglycylglycylglycylglycylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C100 H143 N21 O32 S

SR CF

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 50 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223119-22-0 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-3-cyclohexyl-D-alanylglycylglycylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C101 H151 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

PAGE 1-A

2 REFERENCES IN FILE CA (1907 TO DATE) 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 51 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223119-13-9 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-3-cyclohexyl-L-alanylglycylglycylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C101 H151 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

PAGE 1-A

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 52 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223119-07-1 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-2-cyclohexylglycylglycylglycylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C100 H149 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

PAGE 1-A

PAGE 2-C



1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 130:297001 1:

L10 ANSWER 53 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223119-00-4 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-D-leucylglycylglycylglycyl- β -alanyl-L- α -aspartyl-L-tyrosyl-L- α -glutamyl-L-prolyl-L-isoleucyl-L $prolyl-L-\alpha-glutamyl-L-\alpha-glutamyl-L-alanyl-3-cyclohexyl-L-$

alanyl- (9CI) (CA INDEX NAME)

PROTEIN SEQUENCE; STEREOSEARCH FS

MF C98 H147 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

PAGE 1-A

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 54 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223118-88-5 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-L-leucylglycylglycylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C98 H147 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE

1: 132:262009

REFERENCE

2: 130:297001

L10 ANSWER 55 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223118-82-9 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-D-isoleucylglycylglycylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C98 H147 N21 O32 S

SR CF

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

-

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 56 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223118-76-1 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-L-isoleucylglycylglycylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C98 H147 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

PAGE 1-A

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 57 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223118-70-5 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-3-methyl-D-valylglycylglycylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C98 H147 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

PAGE 1-A

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE

1: 132:262009

REFERENCE

2: 130:297001

L10 ANSWER 58 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223118-64-7 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-3-methyl-L-valylglycylglycylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C98 H147 N21 O32 S

SR CF

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 59 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223118-59-0 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-D-valylglycylglycylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C97 H145 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 60 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223118-52-3 REGISTRY

D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-CN (2R)-2-piperidinecarbonyl-L-valylglycylglycylglycyl- β -alanyl-L- α -aspartyl-L-tyrosyl-L- α -glutamyl-L-prolyl-L-isoleucyl-Lprolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-Lalanyl- (9CI) (CA INDEX NAME) PROTEIN SEQUENCE; STEREOSEARCH

FS

MF C97 H145 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

PAGE 1-A

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 61 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223118-41-0 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-D-methionylglycylglycylglycyl- β -alanyl-L- α -aspartyl-L-tyrosyl-L- α -glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L- α -glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C97 H145 N21 O32 S2

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 62 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223118-31-8 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-L-methionylglycylglycylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C97 H145 N21 O32 S2

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

PAGE 1-A

HO2C
R
CO2H

O
NH
O
HO2C
S
N
H
S
N
H
S
N
H
S
N
H
S
N
H
S
Me
Et

PAGE 1-C

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

1: 132:262009

REFERENCE

2: 130:297001

L10 ANSWER 63 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223118-20-5 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-3-mercapto-D-valylglycylglycylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C97 H145 N21 O32 S2

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 64 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223118-14-7 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-3-mercapto-L-valylglycylglycylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C97 H145 N21 O32 S2

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1:

l: 132:262009

REFERENCE

2: 130:297001

L10 ANSWER 65 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223118-04-5 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-L-cysteinylglycylglycylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C95 H141 N21 O32 S2

SR CA

LC STN Files: CA, CAPLUS

PAGE 1-A

1 REFERENCES IN FILE CA (1907 TO DATE)
1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 130:297001

L10 ANSWER 66 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223117-95-1 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-D-norleucylglycylglycylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C98 H147 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

PAGE 1-A

HO2C
R
CO2H

O
NH
O
HO2C
S
N
H
S
N
H
S
Me
Et

PAGE 1-C

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 67 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN RN 223117-89-3 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl(2R)-2-piperidinecarbonyl-L-norleucylglycylglycylglycyl-β-alanyl-Lα-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-Lprolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-Lalanyl- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C98 H147 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

2 REFERENCES IN FILE CA (1907 TO DATE) 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

ANSWER 68 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN 223117-81-5 REGISTRY L10

RN

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-D-norvalylglycylglycylglycyl-β-alanyl-L- $\alpha \hbox{-aspartyl-L-tyrosyl-L-}\alpha \hbox{-glutamyl-L-prolyl-L-isoleucyl-L-}$ prolyl-L-\alpha-glutamyl-L-\alpha-glutamyl-L-alanyl-3-cyclohexyl-Lalanyl- (9CI) (CA INDEX NAME)

PROTEIN SEQUENCE; STEREOSEARCH FS

MF C97 H145 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

PAGE 1-A

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 69 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223117-75-7 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-L-norvalylglycylglycylglycylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C97 H145 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE

1: 132:262009

REFERENCE

2: 130:297001

L10 ANSWER 70 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223117-70-2 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-(2R)-2-aminobutanoylglycylglycylglycyl- β -alanyl-L- α -aspartyl-L-tyrosyl-L- α -glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L- α -glutamyl-L- α -glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C96 H143 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

PAGE 1-A

2 REFERENCES IN FILE CA (1907 TO DATE)
2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 71 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 223117-64-4 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-(2S)-2-aminobutanoylglycylglycylglycyl- β -alanyl-L- α -aspartyl-L-tyrosyl-L- α -glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L- α -glutamyl-L- α -glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

PROTEIN SEQUENCE; STEREOSEARCH

FS PROTEIN SEQUENCE; S MF C96 H143 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

PAGE 1-A

2 REFERENCES IN FILE CA (1907 TO DATE) 2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

132:262009 REFERENCE 1:

130:297001 REFERENCE 2:

REGISTRY COPYRIGHT 2004 ACS on STN ANSWER 72 OF 82 L10

223117-53-1 REGISTRY RN

D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-CN (2R)-2-piperidinecarbonyl-2-methylalanylglycylglycylglycyl-β-alanyl-L- $\alpha - \texttt{aspartyl-L-tyrosyl-L-} \alpha - \texttt{glutamyl-L-prolyl-L-isoleucyl-L-}$ $prolyl-L-\alpha-glutamyl-L-\alpha-glutamyl-L-alanyl-3-cyclohexyl-1-alanyl-3-cyclohexyl-1-alanyl$ alanyl- (9CI) (CA INDEX NAME)

PROTEIN SEQUENCE; STEREOSEARCH

FS C96 H143 N21 O32 S MF

SR

STN Files: CA, CAPLUS LC

Absolute stereochemistry.

PAGE 1-A

PAGE 1-C

2 REFERENCES IN FILE CA (1907 TO DATE)

2 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

L10 ANSWER 73 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN RN 197519-06-5 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-D-alanylglycylglycylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C95 H141 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

REFERENCE 3: 127:316126

L10 ANSWER 74 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 197518-27-7 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycylglycylglycylglycyl-N-methyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C95 H141 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

PAGE 1-A

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 127:316126

L10 ANSWER 75 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 197518-19-7 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycylalanylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-

(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH MF C95 H141 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

PAGE 1-C

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 127:316126

L10 ANSWER 76 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 197518-17-5 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-N-methylglycylglycyl- β -alanyl-L- α -aspartyl-L-tyrosyl-L- α -glutamyl-L-prolyl-L-isoleucyl-L-

prolyl-L- α -glutamyl-L- α -glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME) PROTEIN SEQUENCE; STEREOSEARCH

FS

C95 H141 N21 O32 S MF

SR

STN Files: LCCA, CAPLUS

Absolute stereochemistry.

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 127:316126

L10 ANSWER 77 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 197518-12-0 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylalanylglycylglycylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C95 H141 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

PAGE 1-A

HO2C
R
O
NH
O
HO2C
O
H
S
N
H
Me
O
HO2C
S
N
H
S
Me
Et

PAGE 1-B

PAGE 1-C

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 127:316126

L10 ANSWER 78 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 197518-11-9 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-N-methylglycylglycylglycylglycylglycyl- β -alanyl-L- α -aspartyl-L-tyrosyl-L- α -glutamyl-L-prolyl-L-isoleucyl-L-

prolyl-L- α -glutamyl-L- α -glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME) PROTEIN SEQUENCE; STEREOSEARCH

FS

C95 H141 N21 O32 S MF

SR CA

STN Files: CA, CAPLUS LC

Absolute stereochemistry.

1 REFERENCES IN FILE CA (1907 TO DATE)

1 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 127:316126

L10 ANSWER 79 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 197518-08-4 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycyl-D-alanylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C95 H141 N21 O32 S

SR CF

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

PAGE 1-B

PAGE 1-C

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

REFERENCE 3: 127:316126

L10 ANSWER 80 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 197518-07-3 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-

(2R)-2-piperidinecarbonylglycylglycyl-L-alanylglycyl- β -alanyl-L- α -aspartyl-L-tyrosyl-L- α -glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-a-glutamyl-L-a-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl- (9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C95 H141 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

REFERENCE 3: 127:316126

L10 ANSWER 81 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 197518-06-2 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonyl-L-alanylglycylglycylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C95 H141 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

PAGE 1-A

PAGE 1-B

=

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001 '

REFERENCE 3: 127:316126

L10 ANSWER 82 OF 82 REGISTRY COPYRIGHT 2004 ACS on STN

RN 197518-05-1 REGISTRY

CN D-Glutamic acid, N2-[[4-(1,1-dimethylethyl)phenyl]sulfonyl]-L-arginyl-(2R)-2-piperidinecarbonylglycylglycylglycylglycylglycyl-β-alanyl-L-α-aspartyl-L-tyrosyl-L-α-glutamyl-L-prolyl-L-isoleucyl-L-prolyl-L-α-glutamyl-L-alanyl-3-cyclohexyl-L-alanyl-(9CI) (CA INDEX NAME)

FS PROTEIN SEQUENCE; STEREOSEARCH

MF C94 H139 N21 O32 S

SR CA

LC STN Files: CA, CAPLUS

RELATED SEQUENCES AVAILABLE WITH SEQLINK

Absolute stereochemistry.

PAGE 1-A

3 REFERENCES IN FILE CA (1907 TO DATE)

3 REFERENCES IN FILE CAPLUS (1907 TO DATE)

REFERENCE 1: 132:262009

REFERENCE 2: 130:297001

REFERENCE 3: 127:316126